

Data-Driven Safety Quantification using Infinite-Dimensional Robust Convex Optimization

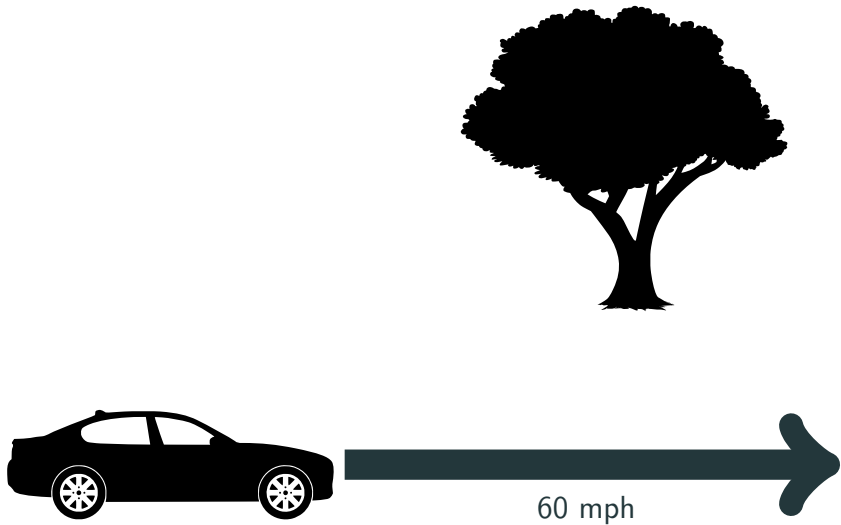
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MSL Lab Meeting

May 19, 2023



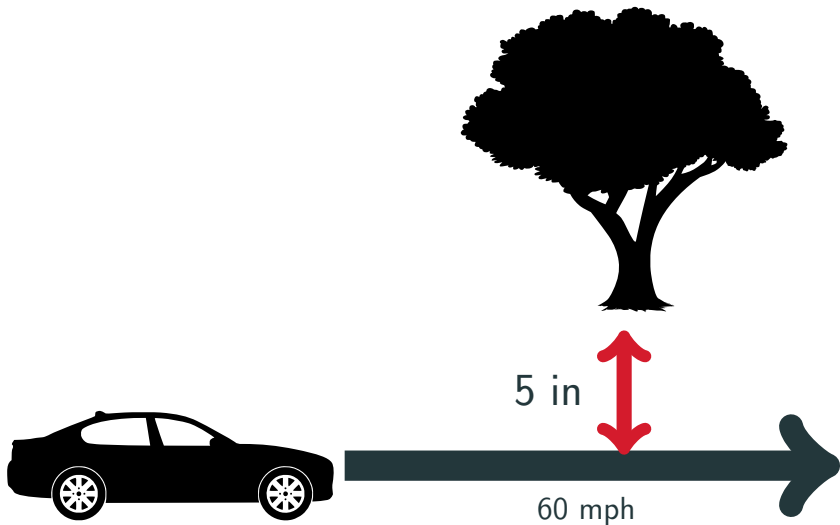
Safety Example



Safety Example (Barrier/Density Function)

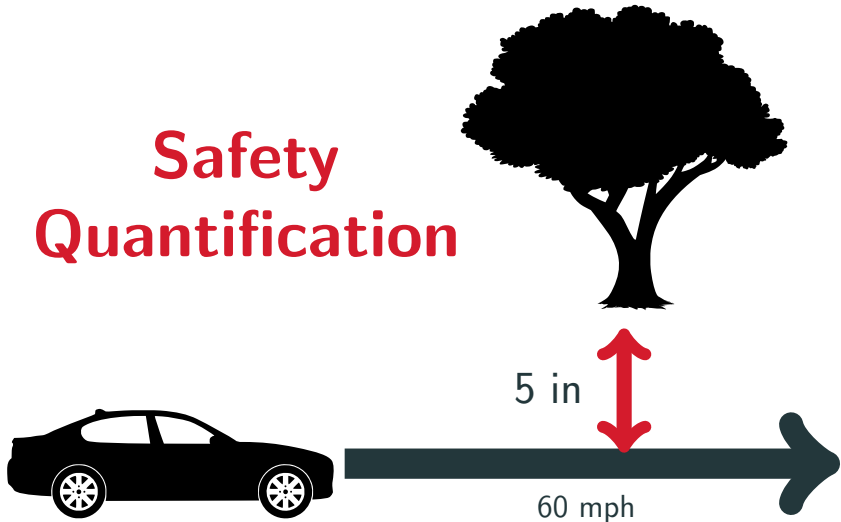


Safety Example (Distance Estimate)



Safety Example (Distance Estimate)

Safety Quantification



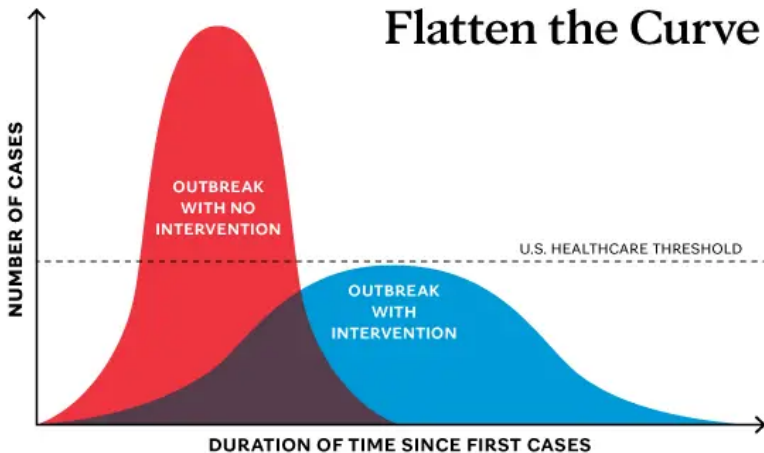
Safety Example (Crash Control Effort)

Safety Quantification



Motivation: Epidemic

Flatten the Curve

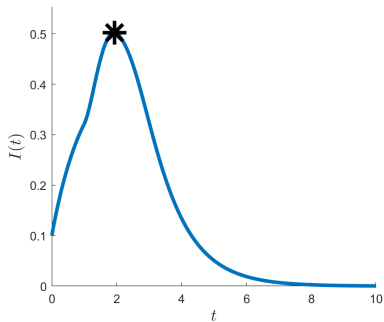


Adapted from CDC

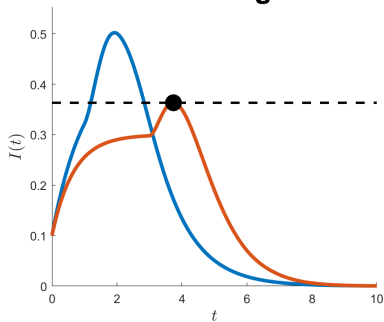
Image credit to Mayo Clinic News Network

Problems Covered

Peak Estimation



Peak-Minimizing Control



Flow of Presentation

Review peak estimation problem and SOS methods

Observe common pattern (peak, distance, crash):

- Input-affine dynamics
- Semidefinite-representable uncertainty

Use structure to simplify Lie derivative constraint

Apply method data-driven systems analysis

Peak and Sum-of-Squares Background

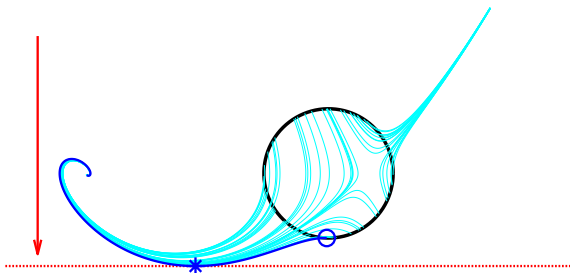
Peak Estimation Problem

Find maximum value of $p(x)$ along trajectories

$$P^* = \sup_{t, x_0 \in X_0} p(x(t))$$

$$\dot{x}(t) = f(t, x(t)) \quad t \in [0, T]$$

$$x(0) = x_0 \in X_0$$



$$\dot{x} = [x_2, -x_1 - x_2 + x_1^3/3]$$

Peak Function Program

Infinite dimensional linear program (Cho, Stockbridge, 2002)

Uses auxiliary function $v(t, x)$

$$d^* = \inf_{\gamma \in \mathbb{R}} \gamma \quad (1a)$$

$$\gamma \geq v(0, x) \quad \forall x \in X_0 \quad (1b)$$

$$\mathcal{L}_f v(t, x) \leq 0 \quad \forall (t, x) \in [0, T] \times X \quad (1c)$$

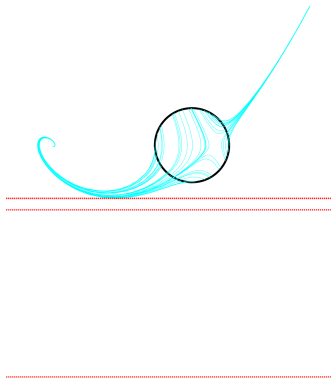
$$v(t, x) \geq p(x) \quad \forall (t, x) \in [0, T] \times X \quad (1d)$$

$$v \in C^1([0, T] \times X) \quad (1e)$$

Lie Derivative $\mathcal{L}_f v(t, x) = \partial_t v + f(t, x) \cdot \nabla_x v$

$P^* = d^*$ holds if $[0, T] \times X$ is compact, f Lipschitz

Peak Estimation Example Bounds



Converging bounds to min. $x_2 = -0.5734$ (moment-SOS)

Box region $X = [-2.5, 2.5]$, time $t \in [0, 5]$

Max. PSD size: $\binom{(n+1)+(d+\lfloor \deg f/2 \rfloor)}{n+1}$ (Fantuzzi, Goluskin, 2020)

Sum-of-Squares Method

Every $c \in \mathbb{R}$ satisfies $c^2 \geq 0$

Sufficient: $q(x) \in \mathbb{R}[x]$ nonnegative if $q(x) = \sum_i q_i^2(x)$

Exists $v(x) \in \mathbb{R}[x]^s$, Gram matrix $Z \in \mathbb{S}_+^s$ with $q = v^T Z v$

Sum-of-Squares (SOS) cone $\Sigma[x]$

$$\begin{aligned} & x^2 y^4 - 6x^2 y^2 + 10x^2 + 2xy^2 + 4xy - 6x + 4y^2 + 1 \\ &= (x + 2y)^2 + (3x - 1 - xy^2)^2 \end{aligned}$$

Motzkin Counterexample (nonnegative but not SOS)

$$x^2 y^4 + x^4 y^2 - x^2 y^2 + 1$$

Sum-of-Squares Method (cont.)

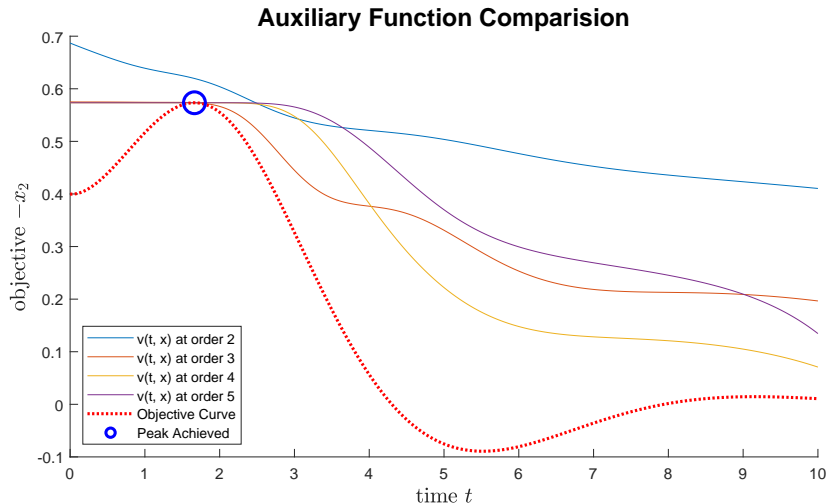
Putinar Positivstellensatz (Psatz) nonnegativity certificate over set $\mathbb{K} = \{x \mid g_i(x) \geq 0, h_j(x) = 0\}$:

$$q(x) = \sigma_0(x) + \sum_i \sigma_i(x)g_i(x) + \sum_j \phi_j(x)h_j(x) \\ \exists \sigma_0(x) \in \Sigma[x], \quad \sigma_i(x) \in \Sigma[x], \quad \phi_j \in \mathbb{R}[x]$$

Psatz at degree $2d$ is an SDP, monomial basis: $s = \binom{n+d}{d}$

Archimedean: $\exists R \geq 0$ where $R - \|x\|_2^2$ has Psatz over \mathbb{K}

Auxiliary Evaluation along Optimal Trajectory



Optimal $v(t, x)$ should be constant until peak is achieved

Peak Estimation with Uncertainty

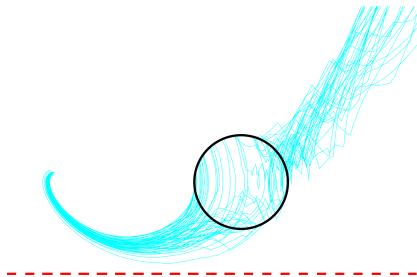
Dynamics $\dot{x} = f(t, x(t), w(t))$

Uncertain process $w(t) \in W, \forall t \in [0, T]$

Time-dependent $w(\cdot)$ with no continuity assumptions

$$\mathcal{L}_{f(t,x,w)} v(t, x) \leq 0 \quad \forall (t, x, w) \in \forall [0, T] \times X \times W$$

System with Uncertainty Example

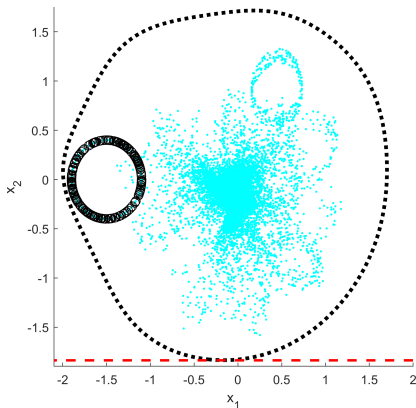


$$\dot{x}(t) = [x_2(t), -x_1 w(t) - x_2(t) + x_1(t)^3/3]$$
$$w(t) \in [0.5, 1.5], \text{ no continuity}$$

(Miller, Henrion, Sznaier, Korda, 2021)

Other types of Uncertainty Structures

- Switching Uncertainty
- Polytopic Restriction
- Slew-Rate Bounded
- Discrete-Time
- Stochastic



Discrete dynamics with switching
and time-dependent uncertainty

Robust Counterparts

Assumptions

Set $[0, T] \times X$ is compact

Uncertainty W is compact and convex

Dynamics $f(t, x, w)$ are Lipschitz in $[0, T] \times X$

Input-affine $f(t, x, w) = f_0(t, x) + \sum_{\ell=1}^L w_{\ell} f_{\ell}(t, x)$

Robust Counterpart Example: Box

(Ben-Tal, Nemirovskii, “Robust Optimization” 2009)

Original β -feasible problem with unknown $\|w\|_\infty \leq 1$

$$\forall w : \quad a_0^T \beta + \sum_{\ell=1}^L w_\ell a_\ell^T \beta \leq b_0 + \sum_{\ell=1}^L w_\ell b_\ell \quad (2)$$

Equivalent program with w eliminated:

$$\max_{\|w\|_\infty \leq 1} \left(\sum_{\ell=1}^L w_\ell [a_\ell^T \beta - b] \right) \leq b_0 - a_0^T \beta \quad (3a)$$

$$\sum_{\ell=1}^L |a_\ell^T \beta - b| \leq b_0 - a_0^T \beta \quad (3b)$$

Semidefinite-Representable (SDR) Set

Build up uncertainty set W using

K_s	Cone
λ_s	Lifting variable
(A_s, G_s, e_s)	Constraint description

Form the intersection

$$W = \cap_s \{ \exists \lambda_s \in \mathbb{R}^{q_s} : A_s w + G_s \lambda_s + e_s \in K_s \}$$

SDR: All $K_s \subseteq$ PSD cone (projections of spectahedra)

Robust Counterparts (General)

Original problem with SDR uncertainty

$$\forall w \in W : \quad a_0^T \beta + \sum_{\ell=1}^L w_{\ell} a_{\ell}^T \beta \leq b_0 + \sum_{\ell=1}^L w_{\ell} b_{\ell}$$

Robust counterpart (sufficient condition)

$$\begin{aligned} \sum_{s=1}^{N_s} e_s^T \zeta_s + a_0^T \beta &\leq b_0 \\ G_s^T \zeta_s &= 0 & \forall s = 1..N_s \\ \sum_{s=1}^{N_s} (A_s^T \zeta_s)_{\ell} + a_{\ell}^T \beta &= b_{\ell} & \forall \ell = 1..L \\ \zeta_s &\in K_s^* & \forall s = 1..N_s. \end{aligned}$$

Nonconservative if (K convex, pointed, non-polyhedral Slater)

Robust Counterparts for Lie Constraint

Original **strict** constraint

$$\mathcal{L}_f v(t, x, w) < 0 \quad \forall (t, x, w) \in [0, T] \times X \times W$$

Specific with $a_0, a_\ell = 0$, $b_0 = \mathcal{L}_{f_0} v$, $b_\ell = f_\ell \cdot \nabla_x v$

Robust counterpart with multipliers ζ

$$\mathcal{L}_{f_0} v(t, x) + \sum_{s=1}^{N_s} e_s^T \zeta_s(t, x) < 0 \quad \forall [0, T] \times X$$

$$G_s^T \zeta_s(t, x) = 0 \quad \forall s = 1..N_s$$

$$\sum_{s=1}^{N_s} (A_s^T \zeta_s(t, x))_\ell + f_\ell(t, x) \cdot \nabla_x v(t, x) = 0 \quad \forall \ell = 1..L$$

$$\zeta_s(t, x) \in K_s^* \quad \forall s = 1..N_s$$

Conditions for Nonconservatism

Strict robust Lie constraint nonconservative if:

1. K_s convex, pointed, non-polyhedral Slater
2. $[0, T] \times X$ is compact
3. (A_s, G_s) constant in (t, x)
4. (f_0, f_ℓ, e_s) continuous in (t, x)

Peak Decomposed Program

Example: Polytopic uncertainty $W = \{w \mid Aw \leq b\}$

Only the Lie Derivative constraint changes

$$d^* = \min_{\gamma \in \mathbb{R}} \gamma$$

$$\gamma \geq v(0, x) \quad \forall x \in X_0$$

$$\mathcal{L}_{f_0} v(t, x) + b^T \zeta(t, x) \leq 0 \quad \forall (t, x) \in [0, T] \times X$$

$$(A^T)_\ell \zeta(t, x) = (f_\ell \cdot \nabla_x) v(t, x) \quad \forall \ell = 1..L$$

$$v(t, x) \geq p(x) \quad \forall (t, x) \in [0, T] \times X$$

$$v(t, x) \in C^1([0, T] \times X)$$

$$\zeta_k(t, x) \in C_+([0, T] \times X) \quad \forall k = 1..m$$

Applicable to any SDR W

Complexity and Input-Affine Structure

Assume input-affine $f(t, x, w) = f_0(t, x) + \sum_{\ell=1}^L w_{\ell} f_{\ell}(t, x)$

Size of largest PSD matrix in degree- d SDP:

$$\text{Original} \quad \binom{1+n+L+d+\lceil \deg(f)/2 \rceil - 1}{1+n+L} = \binom{18}{13} = 8568$$

$$\text{Decomposed} \quad \binom{1+n+d+\lceil \deg(f)/2 \rceil - 1}{1+N_x} = \binom{8}{3} = 56$$

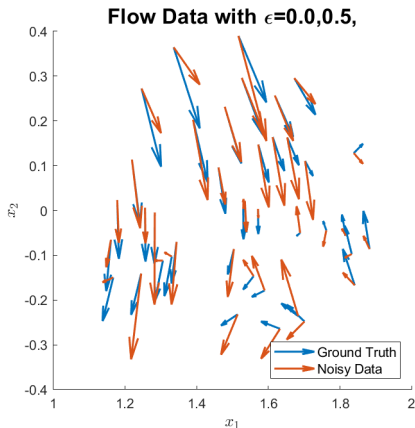
Values with $d = 4$, $L = 10$, $n = 2$

W polytope with 33 faces, 7534 vertices

Data-Driven Analysis

Sampling: Flow System

Data $\mathcal{D} = \{(t_j, x_j, \dot{x}_j)\}_j$ under mixed L_∞ -bounded noise



$$\dot{x} = [x_2, -x_1 - x_2 + x_1^3/3]$$

Dynamics Model

Given data \mathcal{D} , budget ϵ , system model $\{f_0, f_\ell\}$

Parameterize ground truth F by functions in dictionary

$$\dot{x}(t) = f(t, x, w) = f_0(t, x) + \sum_{\ell=1}^L w_\ell f_\ell(t, x)$$

Ground truth satisfies corruption $J(w^*) \leq \epsilon$

L_∞ example: $J(w) = \max_j \|f(t_j, x_j, w) - \dot{x}_j\|_\infty$

Peak Estimation Examples

Elliptope Constraint on Input

$$W = \left\{ w \in \mathbb{R}^3 : \begin{bmatrix} 1 & w_1 & w_2 \\ w_1 & 1 & w_3 \\ w_2 & w_3 & 1 \end{bmatrix} \succeq 0 \right\}.$$

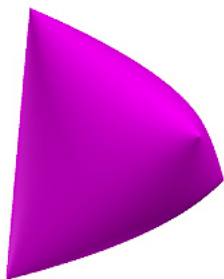
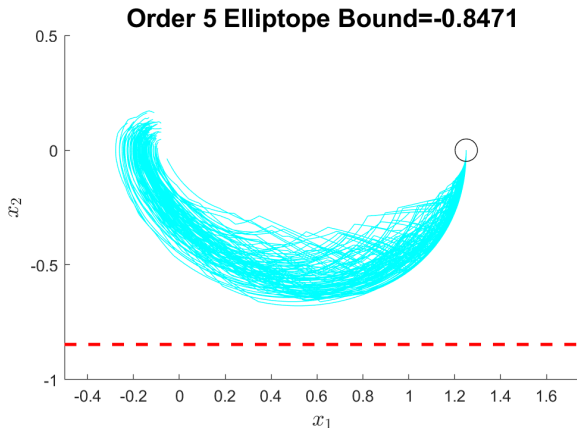


Image credit: Dattoro

Peak Estimation Example (Flow-Elliptope)

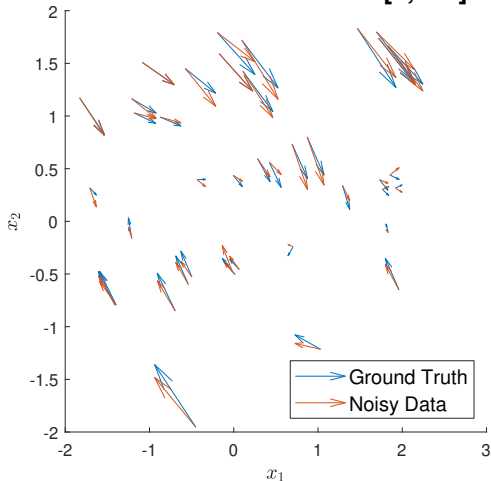


$$f(t, x, w) = \begin{bmatrix} x_2 \\ -x_1 - x_2 + x_1^3/3 + w_1x_1 + w_2x_1x_2 + w_3x_3 \end{bmatrix}$$

Uses polynomial matrix inequalities of size 3×3

Peak Estimation Example (Flow)

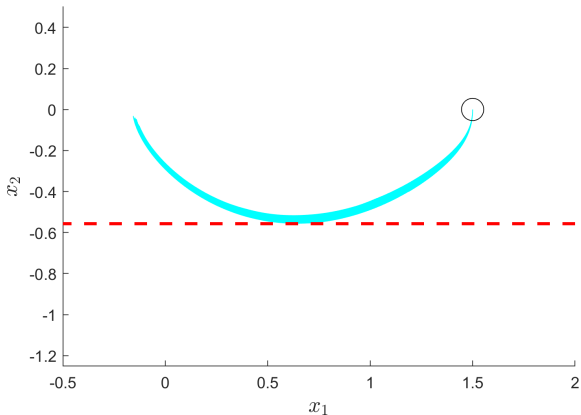
40 observations with $\epsilon=[0, 0.5]$



$$\dot{x} = [x_2, -x_1 - x_2 + x_1^3/3], \quad T = 5$$

Peak Estimation Example (Flow)

Order 4 bound = 0.557

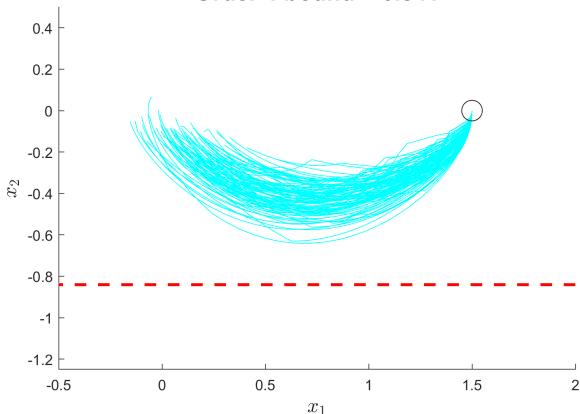


$$\dot{x} = [x_2, -wx_1 - x_2 + x_1^3/3]$$

$$L = 1, m = 80 \text{ (2 nonredundant)}$$

Peak Estimation Example (Flow)

Order 4 bound = 0.841



$$\dot{x} = [x_2, \text{cubic}(x_1, x_2)]$$

$L = 10, m = 80$ (33 nonredundant)

Distance Estimation

Unsafe set X_u , point-set distance $c(x; X_u) = \inf_{y \in X_u} c(x, y)$

$$P^* = \sup_{t, x_0 \in X_0, w} -c(x(t \mid x_0); X_u)$$

$$\dot{x}(t) = f(t, x(t), w(t)) \quad \forall t \in [0, T], \quad x(0) = x_0$$

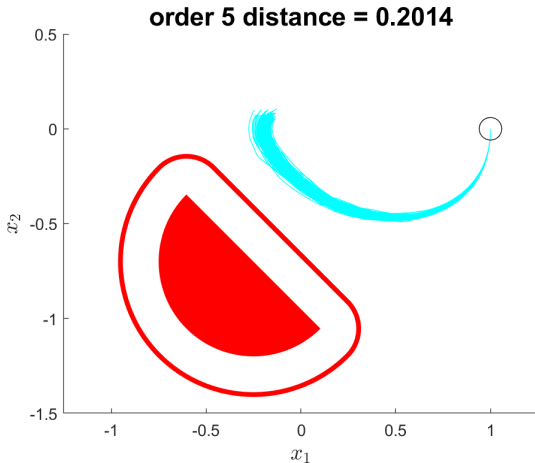
Polynomial-expressible constraints with $\phi(x)$

$$v(t, x) \geq \phi(x) \quad \forall (t, x) \in [0, T] \times X$$

$$\phi(x) \geq -c(x, y) \quad \forall (x, y) \in X \times X_u$$

No change to Lie derivative $\mathcal{L}_f v(t, x, w) \leq 0$

Distance Estimation Example (Flow)



$$\dot{x} = [x_2, \text{cubic}(x_1, x_2)]$$

$$L = 10, m = 80 \text{ (33 nonredundant)}$$

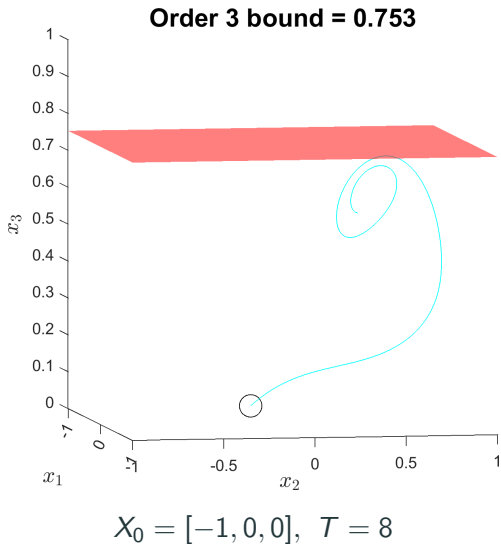
Peak Estimation Example (Twist)

Dynamics model:

$$\dot{x}_i = A_{ij}x_j - B_{ij}(4x_j^3 - 3x_j)$$

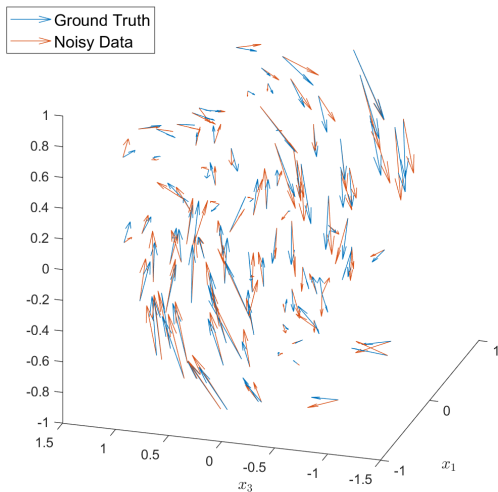
$$A = \begin{bmatrix} -1 & 1 & 1 \\ -1 & 0 & -1 \\ 0 & 1 & -2 \end{bmatrix}$$

$$B = \begin{bmatrix} -\frac{1}{2} & 0 & -\frac{1}{2} \\ 0 & \frac{1}{2} & \frac{1}{2} \\ \frac{1}{2} & \frac{1}{2} & 0 \end{bmatrix}$$



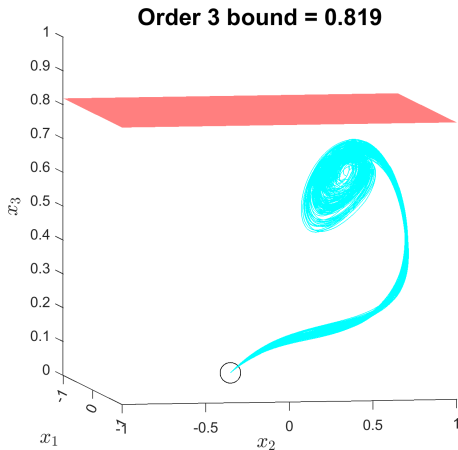
Peak Estimation Example (Twist)

100 Noisy Observations with $\epsilon=0.5$



$$m = 2N_sN_x = 600 \text{ constraints}$$

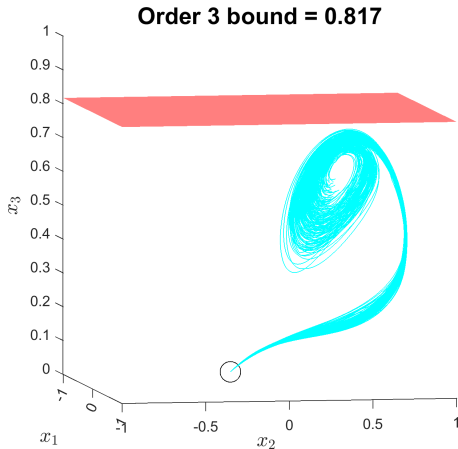
Peak Estimation Example (Twist)



Unknown A , Known B

$$L = 9, \quad m = 600 \text{ (34 nonredundant)}$$

Peak Estimation Example (Twist)

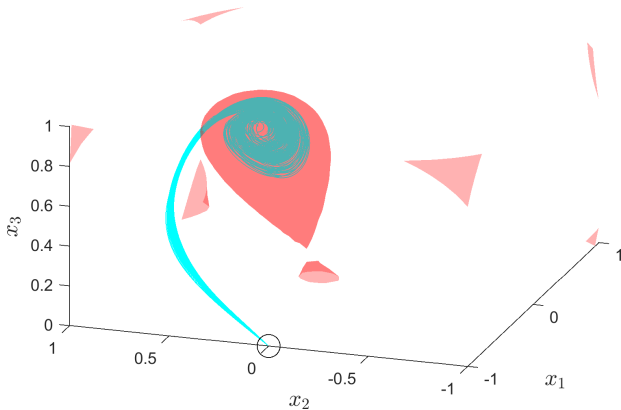


Known A , Unknown B

$$L = 9, \quad m = 600 \text{ (30 nonredundant)}$$

Reachable Set Estimation Example (Twist)

Order 4 volume = 0.756



Unknown A, Known B

$L = 9$, $m = 600$ (34 nonredundant)

Crash-Safety

Crash-Safety

Corruption in L_∞ -bounded setting

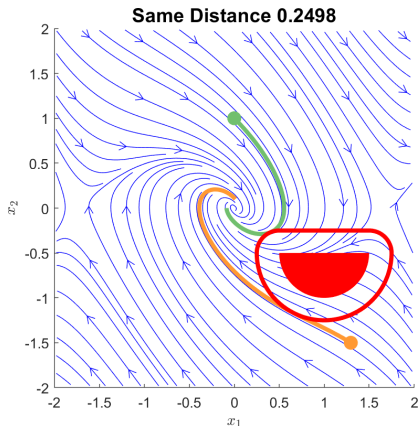
$$\begin{aligned} J(w) &= \max_k \|f_0(t_k, x_k) + \sum_{\ell=1}^L w_\ell f_\ell(t_k, x_k) - y_k\|_\infty \\ &= \max(h - \Gamma w) \quad \text{for some polytope } (\Gamma, h) \end{aligned}$$

How much data corruption is needed to crash?

$$\begin{aligned} Q^* &= \inf_{t, x_0, w} \sup_{t' \in [0, t]} J(w(t')) \\ \dot{x}(t') &= f(t', x(t'), w(t')) \quad \forall t' \in [0, T] \\ x(t \mid x_0, w(\cdot)) &\in X_u \\ w(\cdot) &\in W, \quad t \in [0, T], \quad x_0 \in X_0 \end{aligned}$$

Example Crash-Bounds

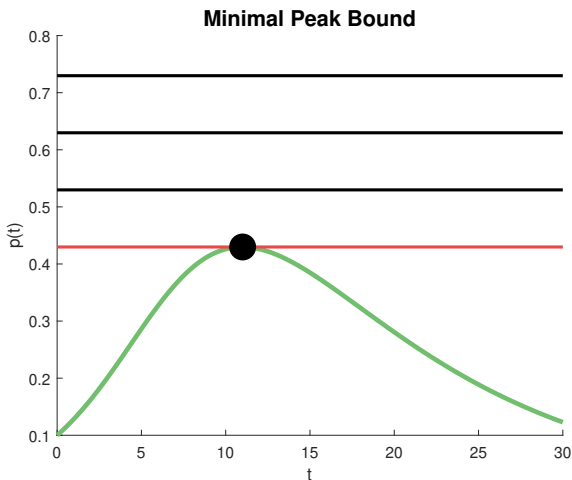
Two trajectories have same distance, different crash-bounds



Green-Top $Q^* = 0.316$, Yellow-Bottom $Q^* = 0.622$

Peak Minimizing Control

Find minimum bound on the maximum p value



Crash-safety is Peak Minimizing Control

Peak-Minimizing Control

Add state $\dot{z} = 0$ (Molina, Rapaport, Ramírez 2022)

$$\begin{aligned} Q_z^* &= \inf_{t, x_0, z, w} z \\ \dot{x}(t') &= f(t', x(t'), w(t')) & \forall t' \in [0, T] \\ \dot{z}(t') &= 0 & \forall t' \in [0, T] \\ J(w(t')) &\leq z & \forall t' \in [0, T] \\ x(t \mid x_0, w(\cdot)) &\in X_u \\ w(\cdot) &\in W, \quad t \in [0, T] \\ x_0 &\in X_0, z \in [0, J_{\max}] \end{aligned}$$

Drive down the z -upper-bound on $J(w)$

Crash-Bound Program

Consistency sets

$$Z = [0, J_{\max}] \quad \Omega = \{(w, z) \in W \times Z : J(w) \leq z\}.$$

Optimal Control Problem with auxiliary $v(t, x, z) \in C^1$

$$d^* = \sup_{\gamma \in \mathbb{R}, v}$$

$$v(0, x, z) \geq \gamma \quad \forall (x, z) \in X_0 \times Z$$

$$v(t, x, z) \leq z \quad \forall (t, x, z) \in [0, T] \times X_u \times Z$$

$$\mathcal{L}_f v(t, x, z, w) \geq 0 \quad \forall (t, x, z, w) \in [0, T] \times X \times \Omega$$

Crash Lie-decomposition

Exploit affine structure of $J(w) = \max_j (h - \Gamma w)_j$

Nonconservatively robustified Lie constraint

$$d^* = \sup_{\gamma \in \mathbb{R}, v}$$

$$v(0, x, z) \geq \gamma$$

$$\forall (x, z) \in X_0 \times Z$$

$$v(t, x, z) \leq z$$

$$\forall (t, x, z) \in [0, T] \times X_u \times Z$$

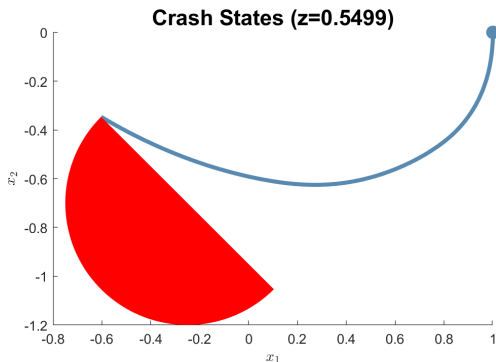
$$\mathcal{L}_{f_0} v - (z \mathbf{1} + h)^T \zeta \geq 0 \quad \forall (t, x, z) \in [0, T] \times X \times [0, J_{\max}]$$

$$(\Gamma^T)_\ell \zeta + f_\ell \cdot \nabla_x v = 0 \quad \forall \ell = 1..L$$

$$\zeta_j \in C_+([0, T] \times X \times Z) \quad \forall j = 1..2nT$$

Data-Driven Flow Crash-Bound

CasADi trajectory matches SOS crash bound



Degree-4 crash bound also 0.5499

True $\epsilon = 0.5$, distance ≈ 0.2014

Flow Crash-Subvalue

Lower bound $q(x)$ for corruption needed to crash ($Q_{\max} < \infty$)

$$J^* = \sup \int_X q(x) dx$$

$$v(0, x, z) \geq q(x)$$

$$\forall (x, z) \in X \times [0, Z_{\max}]$$

$$q(x) \leq Q_{\max}$$

$$\forall x \in X$$

$$z \geq v(t, x, z)$$

$$\forall (t, x, z) \in [0, T] \times X_u \times Z$$

$$\mathcal{L}_f v(t, x, z, w) \geq 0$$

$$\forall (t, x, z, w) \in [0, T] \times X \times \Omega$$

$$v \in C^1([0, T] \times X \times Z)$$

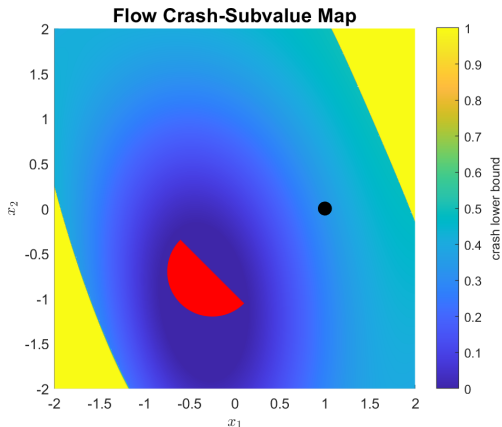
$$q \in C(X)$$

Based on Joint+Marginal optimization (Lasserre, 2010)

Flow Crash-Subvalue

Piecewise-polynomial subvalue

$$q_{1:d}(x) = \max(-l_u(x), \max_{d' \in 1..d} q_{d'}(x))$$



Bound of $0.3399 \leq 0.5499$, but valid everywhere in X

Take-aways

Conclusion

Tractable safety quantification problems

More SOS constraints in fewer variables

Data-driven estimates given semidefinite-bounded noise

Other applications

- Barrier Functions
- Maximum controlled invariant sets
- Hybrid systems
- Set-set (shape) distance estimation
- Distance-maximizing control
- Reachable set estimation

Safety is Important



Quantify using Peak Estimation

Extra Material

Preprocessing: Centering

Chebyshev center c : center of sphere with largest radius in W

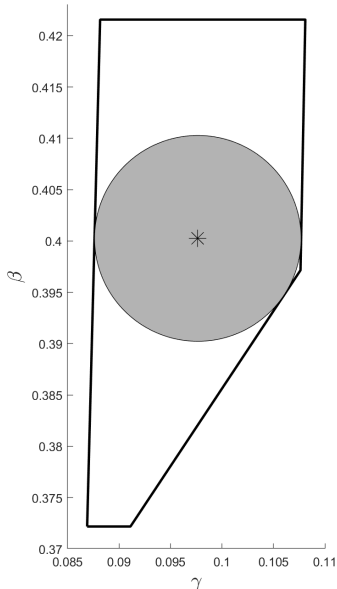
Find through linear programming

$$\max r$$

$$A_k c + r \|A_k\|_2 \leq b_k \quad \forall k$$

$$r \geq 0, c \in \mathbb{R}^L$$

Shifted dynamics $f_0 \leftarrow f_0 + \sum_{\ell=1}^L c_\ell f_\ell$



Preprocessing: Redundancy

Majority of $m = 2N_x N_s$
constraints are often redundant

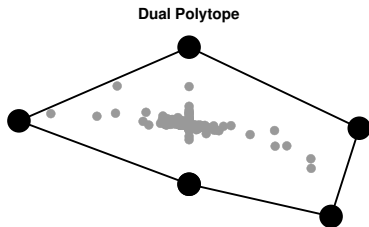
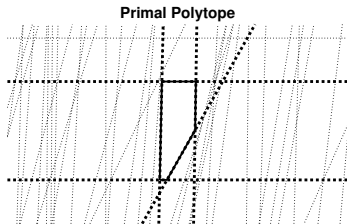
Convex hull of dual polytope:

Time: $\Omega(m \log m + m^{\lfloor L/2 \rfloor})$

Linear program per constraint:

Time: $m \times \tilde{O}(mL + L^3)$

(Jan van den Brand *et. al.* 2020)



Polynomial Matrix Inequalities

SOS method (scalar): $q(x) \geq 0$

Extend to matrices $Q(x) \in \mathbb{S}_{++}^s$

SOS matrix: $Q(x) = R(x)^T R(x) \in \Sigma^s[x]$ for matrix $R(x)$

Gram matrix (PSD) constraint of size $s \binom{n+d}{d}$

Scherer Psatz: nonnegativity over constraint sets